



Structure of Nanoconfined Water

A. D. Trifunac and S. D. Chemerisov

Water, when confined to small spaces, has different structure than bulk water. This implies that water in nanodomains may exhibit different properties that affect processes such as diffusion and reactivity. Water occupies small pores of porous glasses, zeolites, or mesoporous silica materials. The water chemistry in such interfacial systems is relevant to questions that arise when high-level waste glass is exposed to water. Hydrogen gas evolution is a particular concern. There are many other systems including water in biological systems where analogous issues of water structure in nanosize spaces may be important. Hydrogen atoms offer a unique probe of such subtle details of structure and reactivity, and are readily formed when water is subjected to ionizing radiation. The spectroscopic features of hydrogen atoms and their diffusion properties are sensitive to the nanoconfined water structure. In experiments at ANL, hydrogen atoms can be distinguished as they diffuse in different regions of a zeolite. Hydrogen atom diffusion is found to be more facile as the nanodomain size is decreased. Thus water structure becomes less ordered than bulk water with

increasing confinement. Hydrogen atoms "heal" the silica material by reaction with radiation-induced defects rather than reacting to give rise to hydrogen gas as in bulk water.